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DEVELOPMENT OF MONTE CARLO MODEL OF HIGH-ENERGY NUCLEAR INTERACTIONS

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Дальнейшее развитие монте-карловской модели высокоэнергетических ядерных взаимодействий

Монте-карловский программный комплекс CASCADE, предназначенный для расчета неупругих адрон- и ядро-ядерных взаимодействий при энергиях от нескольких десятков МэВ до нескольких десятков ГэВ и для моделирования ядерно-физических процессов, сопровождающих транспорт частиц и ядер в средах, усовершенствован путем включения более детальных моделей распада высоковозбужденных остаточных (послекаскадных) ядер. Результаты расчетов хорошо согласуются с опытом. Вместе с тем наблюдаются некоторые отклонения в распределениях рождающихся легких изотопов, указывающие на необходимость разработки более точных моделей испарения и асимметричного высокоэнергетического деления.

Работа выполнена в Лаборатории информационных технологий ОИЯИ.

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Development of Monte Carlo Model of High-Energy Nuclear Interactions

Monte Carlo code CASCADE for calculation of inelastic hadron- and nucleus–nucleus interactions at energies from several tens of MeV up to several tens of GeV and for modelling of nuclear-physical processes accompanying transport of particles and nuclei in matter is improved due to a more detailed model of decay of highly excited residual (after-intranuclear-cascade) nuclei. Results of calculations are in good agreement with experiment. However, there are some deviations for light isotope production, which prompt the necessity of developing more correct models of evaporation and strong asymmetric high-energy fission.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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INTRODUCTION

Many important applied problems — for example, study of accelerator-driven nuclear reactors for production of energy and transmutation of radioactive waste, design of shielding for accelerators and space vehicles, use of particle beams for cancer therapy, etc. — demand mathematical modeling of high-energy particle transport in media and accompanying physical effects. Experiments in these regions are rather complicated and expensive, so in many cases such calculations are only one way to get information, as the considered systems have a complicated geometrical structure with heterogeneous density. Monte Carlo method is the most convenient one for the calculations allowing one to take into account practically all details of experiments. Several Monte Carlo codes are developed for such investigations, in particular, based on H. Bertini's intranuclear cascade model code LAHET [1] and its generalization LAHET/GEM [2–4], the code CASCADE [5, 6] developed in Dubna with its modifications SONET [6, 7], SHIELD [8], CEM2k+GEM2 [9]. To describe low-energy neutron interactions, all these codes use the multigroup constants tested in reactor physics.

The main difference between LAHET and CASCADE consists in the principally different approach to the description of excited residual (aftercascade) nuclei fission and in distinct models used for calculations of inelastic hadron interactions in the process of intranuclear cascade development. In LAHET and in its improved version LAHET/JEM, masses, charges and energies of fission splinters are sampled using some phenomenological distributions for these quantities (see for example [3]). In this case good or bad agreement of calculations with experiment says nothing on the mechanism of nuclear fission and characterizes only the quantity of the used approximations. Such an approach is worth considering for applied problems, connected with particle transport in matter; however, it is unsufficient for physical investigations. In contrast, the code CASCADE uses a microscopic description of fission based on liquid-drop model [10–12]. By use of fission models the agreement with experimental charge-mass distributions of produced isotopes, as a rule, is somewhat worse, especially for high- and low-mass nuclei (strong asymmetric fission).

In CASCADE, hadron interactions are sampled by means of tables of phenomenological parameters [10, 13] taking into account energy-momentum conservation law and decreasing of intranuclear density due to a knock-out of nucleons [14]. The latter effect is especially important at high energies and in nucleus–nucleus collisions where many intranuclear interactions happened. Decay of a aftercascade nucleus includes three processes: a relaxation of high-excited nucleus, accompanied by a possible emission of nucleons and light fragments, to an equilibrium state; decay of this state due to the competition of particle evaporation and fission; and, finally, hadron and light-fragment evaporation from splinters of fission nucleus may occur if they have enough excitation energy. The relaxation in preequilibrium stage is considered on the basis of the Blann model [15,16]. Monte Carlo modelling of the evaporation and fission is described in the next two sections. It is supposed that the residual several MeV of the excitation are taken by emitted γ quanta. The description of the models of hadron interactions used in LAHET one can find in [1].

Modelling of intranuclear cascades is briefly described in papers [6, 17] and in general terms is closer to the methods used in other transport codes. Cross sections of the hadron–nucleus collisions in our code are calculated based on the compilations of the experimental data [18, 19]. To calculate the nucleus–nucleus cross sections, we use analytical approximations with parameters defined in comparison with experiment [18, 20]. The neutrons with energies less than 10.5 MeV are considered by means of 26-group constants [21]. The use of more detailed constant sets is important for modelling of transmutation processes and isotope distribution in low-energy fission. Due to large ionization losses, low-energy charged particles in intranuclear showers can be considered, in most cases, as stopped. The respective cut-off energies are 2 MeV for π^+ mesons (low-energy π^- mesons are captured by nuclei generating intranuclear cascades), 10 MeV for protons and deuterons, 30 MeV for tritons and 100 MeV/nucleon for all heavier ions. However, for biophysical problems, investigation of radiation damage to microelectronic devices and some other applications, where large radiation damage produced by low-energy particles is important, one must consider lower cut-off energies [17]. Possible decays of π mesons are also taken into account.

The calculations of intranuclear cascades are described in detail in [10,13,14]. The goal of our paper is to describe the improvements of the model for decay of excited residual nuclei (particularly for their fission), which allow one to get better agreement of CASCADE code calculations with experiment and can be applied to other codes being used now.

1. DESCRIPTION OF THE EVAPORATION MODEL

Instead of the simple approximation for Fermi-gas level density

$$\rho(E) = C \exp\left(\sqrt[2]{a(E-\Delta)}\right) \tag{1}$$

with constant value of parameter a used in the previous versions of CASCADE, we use now a more precise expression

$$\rho(E) = C_1(E-\Delta)^{-5/4}a^{-1/4}\,\exp\left(\sqrt[2]{a(E-\Delta)}\right) \tag{2}$$

for the excitation energies $E \geqslant E_b$ and

$$\rho(E) = C_2\,\exp\left(E-E_1\right)/T, \tag{3}$$

if $E < E_b$. The boundary energy $E_b = E_0 + \Delta$, where $E_0 = 2.5 + 150/A_d$ and A_d is the decayed (daughter) nucleus mass number. The parameter $1/T$ is of the form $\sqrt{a/E_o} - 1.5/E_0$ [22, 23] and $E_1 = E_b - T(\log T - 0.25\log a - 1.25\log E_0 + 2\sqrt{aE_0})$. The constant C_2 is defined by the condition of the equality of the densities (2) and (3) at the point $E = E_b$. The pairing energy shift Δ is defined according to the tables [22, 23]. For the level density parameter we use the expression [24–26]

$$a(A_d, Z_d, E) = A_d(S/E)(0.134 - 1.21\cdot 10^{-4}A_d(1-\exp\left(-0.061E\right))). \tag{4}$$

Here A_d and Z_d are the mass and charge numbers of the decayed nucleus, E is the decaying (parent) nucleus excitation energy (MeV), S is the shell correction [22].

The evaporation probability for the particle (or fragment) i is defined by the expression (in units of $\hbar = c = 1$)*

$$P_i = (2/\pi)m_i(2s_i+1)\int\limits_{V_i}^{U_i-B_i}\sigma_i(E)\rho(U_i-B_i-E)EdE, \tag{5}$$

where s_i and m_i are the spin and mass of the evaporated particle. For the binding energy B_i we use the values from the tables [27]). U_i is the excitation energy of the decaying nucleus. The cross section of inverse reaction is defined as

$$\sigma(E) = \pi R^2\alpha(1+\beta/E) \tag{6}$$

with the constants α and β taken from [23] and $R = 1.5(A_i^{1/3} + A_d^{1/3})$, where A_i is the evaporating particle mass number. The Coulomb barrier is of the form

$$V_i = 1.44C_iT_iZ_i(Z-Z_i)/(1.2A_i^{1/3} + 1.7A_d^{1/3})\ [\text{MeV}], \tag{7}$$

where C is the constant proposed by S. Furihota [4] and depends on the charge number of the emitted particle Z_i; A and Z are the mass and charge numbers

*As Monte Carlo sampling uses relative probabilities, the normalization factor, which is common for all evaporation channels and for fission, can be omitted.

of the decaying nucleus. As before, A_d is the mass number of the decayed (daughter) nucleus. Coefficient

$$T_i = \begin{cases} 1/(1+\sqrt{(E/20a_d)}), & E > 200 \text{ MeV}, \\ 1, & E \leqslant 200 \text{ MeV} \end{cases} \tag{8}$$

with the level density parameter a_d takes into account the empirical temperature dependence.

As level density parameter is energy-dependent, the probabilities of evaporation (and fission, see below) are calculated by means of numerical integration instead of customary use of some approximate expressions. Sampling of the energy of a particle emitted by residual nucleus must be done taking into account Eqs. (2)–(8). Such a sampling is rather complicated; however, the calculated; emitted particle energies are close to ones calculated by the use of simple Eq. (1).

In most cases one may restrict oneself to the evaporation of six particles: n, p, d, t, ^{3}He, ^{4}He. The heavier fragments are important only in considering of the isotope production and other particular problems. Calculation of such fragments is time consuming, because one must take into account the emission of fragments in various excited (resonance) states which must be considered as independent states. How to take into account heavy fragments, was shown by S. Furihota [2,4]. Otherwise the light isotope cross sections will be essentially underestimated.

2. SIMULATION OF FISSION

The probability of fission is of the form

$$P_f = \int_0^{U_f - B_f} \rho(U_f - B_f - \Delta_f - E)\, dE, \tag{9}$$

where the fission barrier B_f is defined as the difference of the saddle point and ground-state nucleus mass taking into account the empirical temperature dependence [14, 28]

$$B_f(E) = B_f(0)/(1+\sqrt{E/2A}). \tag{10}$$

The pairing-energy correction is

$$\Delta_f = 14\chi/\sqrt{A} \tag{11}$$

with $\chi = 2$, 1, 0 for even–even, even-odd and odd–even, odd-odd nuclei, respectively.

The probabilities (5), calculated for all taken into account evaporating particles together with fragments, and the fission probability (9) are used for sampling of competition of the reaction channels. Calculations have shown that agreement with experiment becomes better if in the level density parameter $a_f(A,Z,E)$ is taken a little higher than in Eq. (4):

$$a_f = a \left\{ \begin{array}{ll} 1.06253 + 0.93377 \cdot 10^{-2} F^2 - 6.099 \cdot 10^{-4} F^3, & Z \leqslant 85 \\ 1.00887 + 0.8866 \cdot 10^{-2} F^2 - 5.7913 \cdot 10^{-4} F^3, & Z > 85 \end{array} \right. \quad (12)$$

with $F = Z^2/A - 30.893$.

The masses, charges, kinetic and excitation energies of splinters are determined on the basis of Fong statistical theory of fission [10,29]. Calculated splinter excitation energy is $U = \Delta M - D_1 - D_2 - V$. We assume that the deformation energies D_i are described by the liquid-drop model. Coulomb potential is given as

$$V = 1.107 Z_1 (Z - Z_2) / \sum_{i=1,2} (G_{1i} + G_{2i}), \quad (13)$$

where

$$G_{1i} = 1 + \alpha_{2i}(1 - 3\eta_i/5) + \alpha_{3i}(1 - 3\eta_i^2/7) A_i^{1/3}), \quad (14)$$

$$\eta_i = 1.3 A_i^{1/3} \sum_{i=1,2} 1.3 A_i^{1/3} (1 + \alpha_{2i} + \alpha_{3i} - (9/35)\alpha_{2i}\alpha_{3i}). \quad (15)$$

Calculating the difference of the fissioning nucleus and splinter mass defects ΔM, we use their experimental values [27] or, when such values are unknown, the mass defects are defined by means of Cameron mass formula and the correction tables [22].

In order to calculate the properties of the fission fragments we need the total density of quantum states at scission point. In the original Fong theory of fission, the complete equilibrium has been assumed and this density is defined as

$$\Omega(E) = C \int_0^E \exp\left(\sqrt[2]{a_1 + a_2 (E_1 + E_2)}\right) dE_1. \quad (16)$$

However, strong evidence has been found for different thresholds of the symmetric and asymmetric fission components [30, 31], which demonstrate the influence of the saddle point configuration on the fission fragment distribution. The competition of different fission components as a function of the excitation energy has been explained by the temperature dependence of shell effects [31, 32]. It seems that the population of the fission valleys is determined before reaching the scission configuration or that the complete equilibrium does not occur while deciding the fission fragment distribution. This prompts that one must exclude the complete equilibrium condition from Fong theory and take into account separately all partial fragment level densities:

$$\Omega(E) = C \int_0^E \exp\left(\sqrt[2]{a_1(E_1 - \Delta_1)}\right) \exp\left(\sqrt[2]{a_2(E - E_1 - \Delta_2)}\right) dE_1. \quad (17)$$

Here A_i and E_i are splinter mass numbers and excitation energies ($E_2 = E - E_1$), A and E are the mass number and excitation energy of the fissioning compound nuclei and a_i are the level density parameters defined by Eq. (4).

3. COMPARISON WITH EXPERIMENT

Calculated neutron yield, differential and integral spectra of neutrons, are close to the values obtained by means of the previous version of our code and agree with experiment. This can be seen from Tables 1, 2 and Fig. 1, where, as an example, some data for lead and uranium are presented. The above-described improvements practically do not change the distribution of produced heat in the target.

Table 1. **Neutron yield in the lead target with radius R and length L irradiated with protons with energy E**

$R = 5.1$ cm,	$L = 61$ cm		$R = 10.2$ cm,	$L = 61$ cm
E, GeV	Exp. [33, 34]	Theor.	Exp. [35]	Theor.
0.47	8 ± 0.4	7.1	8.7 ± 0.4	7.4
”	6.4 ± 0.3			
0.72	11.8 ± 0.6	12.0	13.9 ± 0.7	14.2
”	11.7 ± 0.4			
0.96	16.6 ± 0.8	17.5	20.3 ± 1.1	20.7
1.47	26.4 ± 1.3	27.9	31.5 ± 1.6	30.9
”	27.5 ± 0.6			

Table 2. **Neutron yield in the uranium target with radius $R = 10.2$ cm and length $L = 61$ cm irradiated with protons with energy E**

E, GeV	Exp. [35]	Theor.
0.47	18.1±0.9	14
0.72	29.1±1.5	28
0.96	40.5±2	38
1.47	56.8±2.8	60

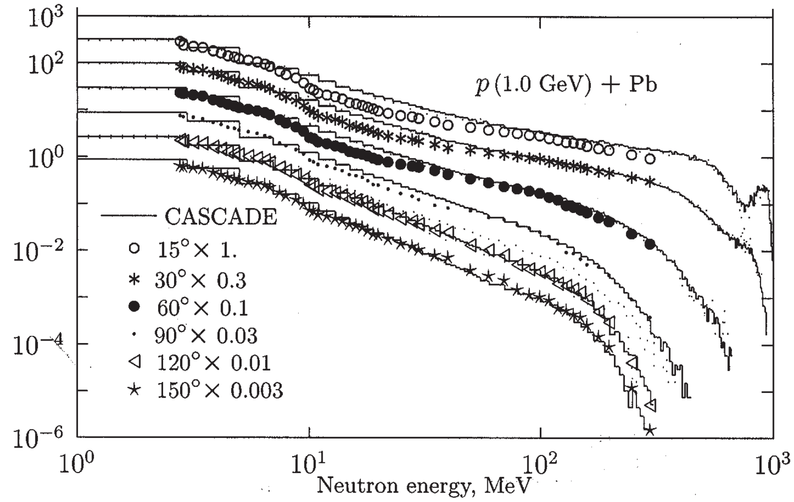

Fig. 1. Energy spectra (mb/MeV/sr) of neutrons created at different angles in the interaction of 1 GeV proton with ^{208}Pb. Experimental points are taken from [36]

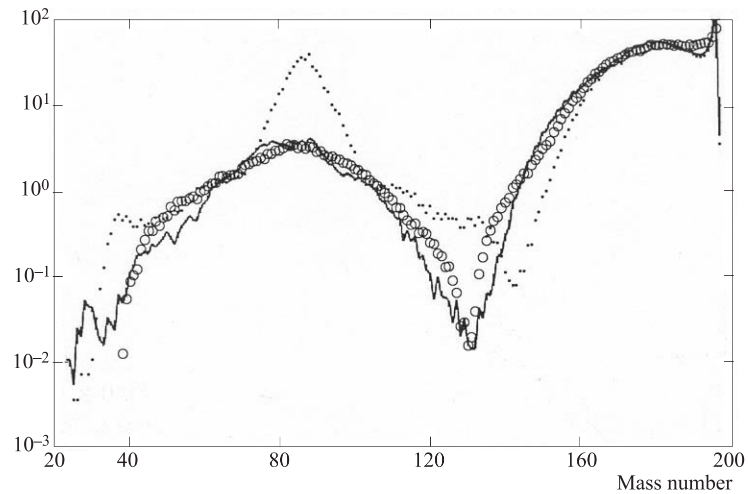

Fig. 2. Mass yield (mb) distribution of isotopes created in inelastic interaction of 0.8 GeV proton with ^{197}Au. Thick and point curves represent calculations by means of the improved version and the old one of the CASCADE code respectively. Open circles represent experimental data [37, 38]

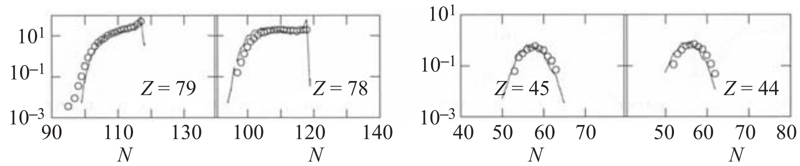

Fig. 3. Yield (mb) distribution of isotopes with charge Z in $p + {}^{197}$Au at $E = 0.8$ GeV. Left panel shows the spallation yield for $Z = 79$ and 78, the right one represents the fission yield for $Z = 45$ and 44, N is the number of neutrons. Experimental points are taken from [37, 38]

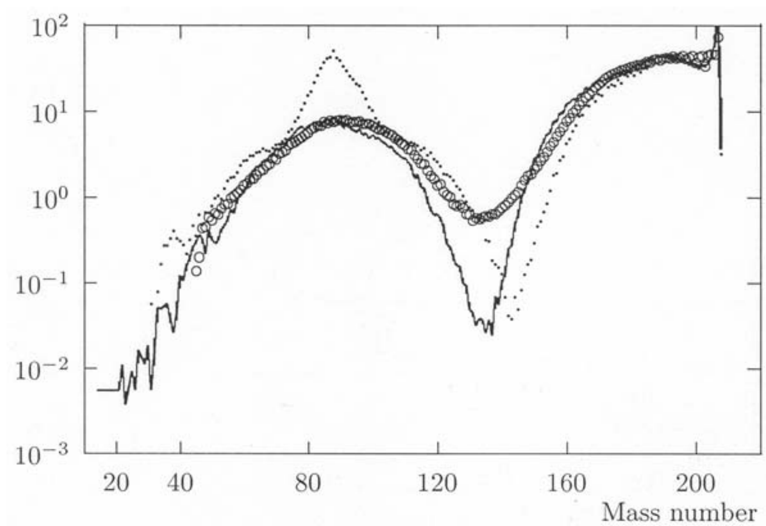

Fig. 4. Mass yield (mb) distribution of isotopes created in inelastic interaction of 1 GeV proton with ^{208}Pb. Notations are similar to those in Fig. 2. Experimental data are taken from [39]

In the previous version of CASCADE, we had a problem with calculation of isotope cross sections. In many cases the experimental and theoretical data differ by a factor of order. The calculated cross sections are changed by the introduced improvements significantly. This is illustrated by Figs. 2–7. In both regions, at the hump created by fission splinters and in the evaporation branch, the agreement with experiment becomes much better. Although it is true that some deviations yet remain. For example, in case of uranium the yield of isotopes with mass numbers $A \simeq 140 - 160$ is essentially less than the experimental one. There are

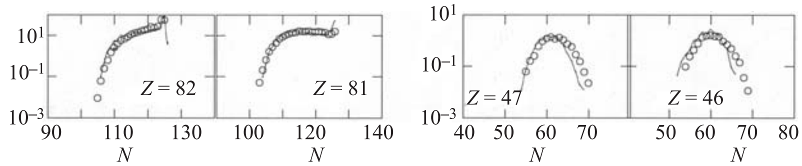

Fig. 5. Yield (mb) distribution of isotopes with charge Z in $p+{}^{208}$Pb at $E=1$ GeV. Left panel shows the spallation yield for $Z=82$ and 81, the right one represents the fission yield for $Z=47$ and 46, N is the number of neutrons. Experimental points are taken from [39]

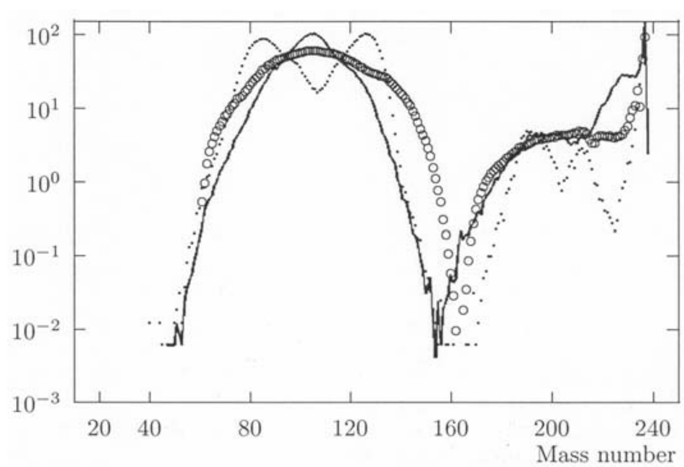

Fig. 6. Mass yield (mb) distribution of isotopes created in inelastic interaction of 1 GeV proton with ^{238}U. Notations are the same as in Fig. 2. Experimental data are taken from [40]

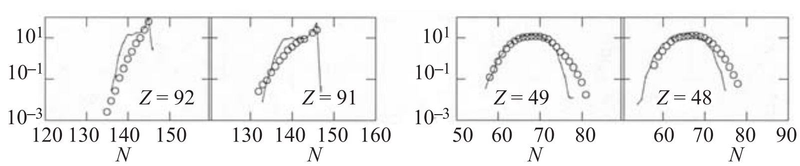

Fig. 7. Yield (mb) distribution of isotopes with charge Z in $p+{}^{238}$U at $E=1$ GeV. Left panel shows the spallation yield for $Z=92$ and 91, the right one represents the fission yield for $Z=49$ and 48, N is the number of neutrons. Experimental points are taken from [40]

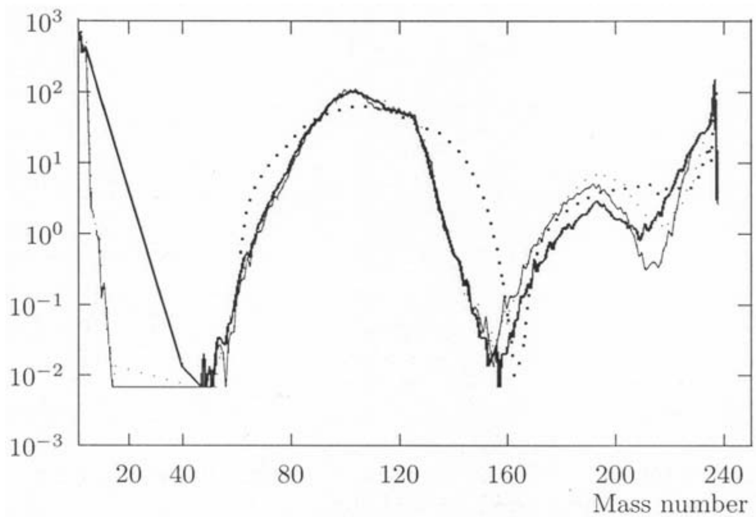

Fig. 8. Calculated isotope mass yield (mb) distribution in collision of 1 GeV proton with ^{238}U at various number of the evaporating particles. Thick curve only six evaporating particles including ^{4}He; thin curve all particles and fragments taken into account including ^{16}C; dotted curve represents particles up to $28_{\rm Mg}$. Points represent the experimental data [40]

some disagreements for light isotopes. The deviations preserve, as can be seen from Fig. 8, even if we take into account the evaporation of heavy fragments. In this region theory needs further development.

CONCLUSIONS

After the improvements of physical models describing the decay , evaporation and fission, of highly excited residual nuclei, the programme complex CASCADE can be used for calculation of the yields, spectral angular distributions of neutron and charge particles created in hadron- and nucleus–nucleus interactions at energies from several tens of MeV up to several tens of GeV and for Monte Carlo modelling of transport of such particles in matter. The code allows one to consider heterogeneous targets with complicated chemical contents. For a better agreement with experiment, one must improve models of decay of highly excited light nuclei and strong asymmetric fission, which are responsible for light isotope production.

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